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The First-Minimum Position of the Wills-Harrison Effective Pair Potential in Liquid Ni

Vladimir Filippov[1,2]

[1)] Ural Federal University, Mira st. 19, 620002 Ekaterinburg, Russia
[2)] Institute of Metallurgy of the Ural Branch of the Russian Academy of Sciences, Amundsen st. 101, 620016 Ekaterinburg, Russia

Abstract

It is found that the position of the first minimum of the Wills-Harrison effective pair potential in the liquid Ni very slightly depends on the probability that not only the diagonal *d-d* couplings between two atoms are possible. This result denotes that the account of the non-diagonal couplings is not such important for the liquid Ni as for both the liquid Fe and liquid Co.

Keywords: Transition metal, Wills-Harrison pair potential, *d*-state coupling

In [1] the Wills-Harrison (WH) model [2] was corrected by means the introduction the probability p that 25 equiprobable *d-d* couplings between two atoms are possible and the probability $(1-p)$ that only 5 equiprobable diagonal couplings are possible.

Recently, we studied the influence of the magnitude p on the position, $r_{\min}$, of the first minimum of the WH effective pair potential, $\varphi_{\mathrm{WH}}(r)$, in the liquid Fe and Co [3, 4]. Here, we fulfil the analogous study for the liquid Ni. Input data (values of parameters and the experimental mean atomic volume, Ω) are listed in Table 1.

One can see from Fig. 1. that the calculated magnitude of the first-minimum position of $\varphi_{\mathrm{WH}}(r)$ is practically constant up to $p = 0.9$. It denotes that the account of the non-diagonal couplings is almost not important in the case of the liquid Ni.

Table 1. Input data for the calculation

r_d (a.u.) [2]	z_s [5]	z_d [5]	R_{C} (a.u.) [5]	a (a.u.) [5]	Ω (a.u.) [6]
1.342	1.4	8.6	1.03	0.207	85.24

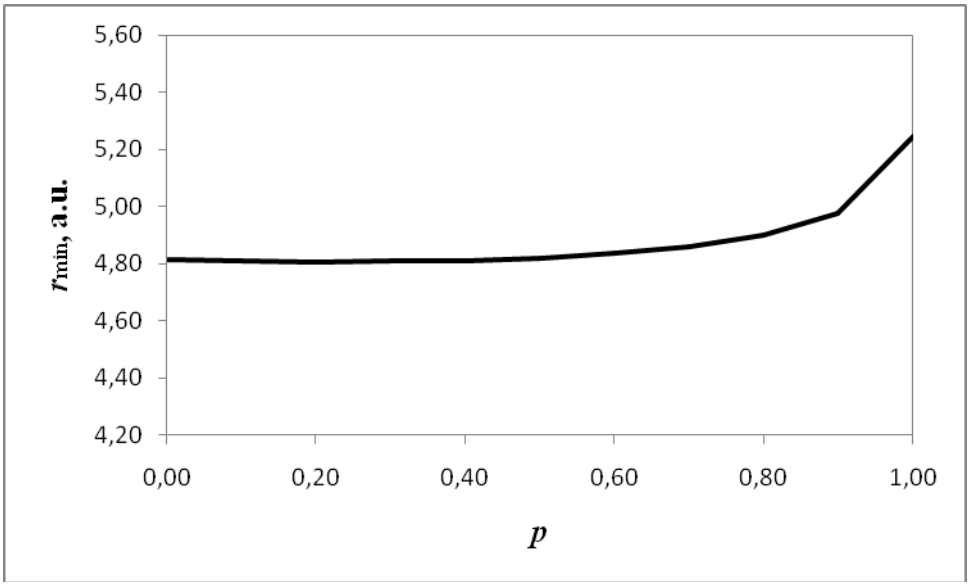

Figure 1. $r_{\min}$ of $\varphi_{\mathrm{WH}}(r)$ in liquid Ni at different p (T=1873K).

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